



chain nodes :

19 20 21 22 24 26 27 28 29 30 31 32 33 41

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

chain bonds :

3-41 6-24 11-41 14-24 19-20 20-21 21-22 26-27 27-28 28-29 30-31 31-32 32-33

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16  
16-17 17-18

exact/norm bonds :

1-2 1-6 2-3 3-4 3-41 4-5 5-6 6-24 11-41 14-24 19-20 20-21 21-22 26-27 27-28  
28-29 30-31 31-32 32-33

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18

G1:C,N

G2:O,N,CH2

G3:[\*1-\*2],[\*3-\*4],[\*5-\*6]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 21:CLASS  
22:CLASS 24:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS  
33:CLASS 41:CLASS